Supporting Information

Authors: Calleri E., Pochetti G., Dossou K.S.S., Laghezza A., Montanari R., Capelli D., Prada E., Loiodice F., Massolini G., Bernier M., Moaddel R.

Title: Resveratrol and its metabolites bind to PPARs

This section contains one table (Table S1) and two figures (Figure S1 and S2)

Table S1. Summary of crystallographic analysis

	resveratrol
space group	C2
cell dimensions *a*, *b*, *c* (Å)	93.72, 63.38, 119.8
monoclinic angle β (deg)	102.9
wavelenght (Å)	1
resolution range (Å)	52.10-2.85
last shell (Å)	3.00-2.85
R_{merge} (%)	7.2 (42.2)[a]
observations	32406 (4415)[a]
unique reflections	13805 (2012)[a]
mean (I)/σ(I)	7.2 (1.8)[a]
completeness	86.2 (86.3)[a]
multiplicity	2.3 (2.2)[a]
structure refinement	
resolution range (Å)	10-2.85
R_{work} (%)	23.7
R_{free} (%)	26.3

a = the values in parenthesis refer to the outer shell

Figure S1. Fo-Fc omit map calculated around the ligand and contoured at 2.5 σ.

Figure S2. Transactivation assay on PPARα and PPARγ of resveratrol and its metabolites at 10 and 25 μM in HepG2 cells.

Fold induction by resveratrol (RV), resveratrol 3-O-sulfate (RVS), resveratrol 3-*O*-glucuronide (RV3G), and resveratrol 4-*O*-glucuronide (RV4G) over vehicle (MeOH 1%) on PPARα and PPARγ as determined by luciferase-based transactivation assays usingrosiglitazone (2 μM) and Wy-14,643 (10 μM) as reference compounds, respectively.

Figure S3. The superposition of PPARγ/resveratrol and PPARα/Wy-14,643 crystal structures